Study on perovskite photovoltaic materials and photovoltaic performance of perovskite solar cells

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Abstract. As a renewable energy, solar energy has aroused people's attention and studies of this issue have become a hot topic throughout the world. How to turn solar energy into electric energy with a relatively better efficiency and lower costs has already become people's new focus. Photovoltaic (PV) cell is such a new device that uses light to generate electricity. Among all of the PV products, the first-generation PV refers to silicon (Si) wafers with a power conversion efficiency (PCE) of 26%. However, these PV cells exhibit relatively high cost, limited conversion efficiency, and high processing cost. While, a new material called perovskite photovoltaic material came into people's eyes. Perovskite materials exhibit variable structures, diversified composition and tubable performance. This material can help to improve the PCE into to a greater level, which is considered as the key performance of PV cells. This work introduces recent developments of halide perovskite and their performances as PV cells.

Keywords: Solar Energy, Perovskite, photovoltaic

1. Introduction

Perovskite is a kind of oxide ceramics with a physical structure of a cube or an octahedral. Calcium titanate, $CaTiO_3$, which was the first perovskite found in perovskite ores, hence its name. Perovskites are usually having a chemical structure of ABX_3[1], an octahedral grid structure, is also called '113 structure', where ion A is usually a rare earth element or an alkaline earth element with a relatively large radius, for example, Ca or Mg; ion B are generally transition elements, like Mn, Co or Fe, and X is usually a halogen anion, like Cl^-, Br^- or I^-. Both ions in A and B can be replaced by other ions that having a similar ionic radius, with its structure almost unchanged. In perovskite structure, the length of the B-X bond can shift as a result of the ionic radius of ion A changing, which can deform the octahedral structure and have a significant impact on the bandgap.

Not only the inorganic ions, perovskite can also consist organic ions, for example, aliphatic or esters, replacing one of the +1 metal ions in the inorganic perovskite. Compared with its inorganic compounds, organic perovskites have some special optical properties, make them more beneficial in UV harvesting. Due to the special structure perovskite has, which concludes high absorption coefficient, long diffusion length, and an optoelectronic property. These properties made it a great development potential in photocatalysis and thermos catalysis. It can be used in the manufacture of solar cells, behave as the substitute of traditional C-Si solar cells.

Since perovskite solar cell exhibit good performance, perovskite photovoltaic materials and their properties in behaving as a solar cell would be discussed in this work.

2. Introductions and properties of different types of Perovskites

2.1. Basic introductions and properties of Lead Halide Perovskite

As was said before, perovskites are usually having a chemical structure of ABX_3[1], this structure also applies to lead halide perovskite. Which is different from other perovskites, the ion B are always a lead ion (Pb); and X is usually a halogen anion, like Cl^-, Br^- or I^-, which is the same as other perovskites.

Lead halide perovskite solar cells, which were first found in 2009, with the join of metal lead, in ten years, which is a very short period of time, its power conversion efficiency registered a significant increase from 3.8% in 2009 to more than 31.4% now. This PCE result is now comparable to the result of single crystalline silicon solar cells, 26.1%, which has a higher cost. One of the inorganic perovskite cases is $CsPbI_3$, in research in 2022, the PCE of $CsPbI_3$ perovskite solar cells reached to a great level of about 20.2%. The research reported that the PCE of a single CsPbI3 device with an absorber layer of 350 nm results in a number of 14.67%. According to the study's findings, the PCE of devices increased to 20.2% and 20.9% when $CsPbI_3$ perovskite solar cells were converted to the 100 nm of $CsPbI_3$ with 700nm of $FAPbI_3$ and 100 nm of $CsPbI_3$ with 700nm of $MAPbI_3$ heterostructures [2].

The organic lead halide perovskite, for example, $CH_3NH_3PbI_3$, has an extremely high UV absorption ability compared with other perovskites, it has been widely used as an UV-absorber in solar cells. However, a suitable band gap for the semiconductor in the solar cells should be about 1.4 eV, organic perovskites, for example, $CH_3NH_3PbBr_3$, has a band gap of about 2.25eV, so by reducing the bandgap of perovskites can help improve the power conversion efficiency. That's also one of the reasons that $CH_3NH_3PbI_3$ has an extremely high UV absorption ability——It has a band gap of 1.66 eV, which is really close to the standard band gap. There are several methods to reduce the bandgaps: by either increasing the B-X-B bond angles or decreasing the electronegativity of negative ions can help reducing the bandgap; In addition, by combining different halogens into the perovskite, the stability and UV absorption ability of the perovskite can be controlled, optimize its power conversion efficiency (PCE).

In research in 2021, $CH_3NH_3PbI_3$ solar cells shows an extremely high power conversion efficiency of 31.4%. In this study, a $CH_3NH_3PbI_3$ light-absorbing layer was positioned between a bi- and tri-layer. The PCE of the solar cell can then be managed by varying the thickness of these layers. Tri-layer, also known as Electron Transport Layer (ETL), is essential to the solar cells' ability to convert light energy into electrical power. Tri-layer has three separate layers, as implied by its name. Titanium dioxide, zinc oxide, and C60 were employed in this research. Each layer in this tri-layer played an important role in improving the PCE. The bi-layer, also known as hole transport material layer (HTL), contains two different layers; Vanadium Pentoxide and Poly (3, 4-Ethylene Dioxythiophene). The research shows that by the decrease of the thickness of the absorb layer (light-harvesting layer), the highest power conversion efficiency result in a value of 31.4%. The study also demonstrates how temperature affects J_{sc}, V_{oc}, FF, and PCE, respectively. Due to the fact that J_{sc} is proportional to incoming light, the increase in J_{sc} with temperature was anticipated. Because series resistances grow at high temperatures, FF decreased as the temperature increased. Between FF and series resistance, there is a linear relationship. The V_{oc} is highly temperature dependent; as temperature rises, it falls as a result of an increase in entropy. In terms of PCE's temperature dependence, the research demonstrates that PCE declines as temperature rises because V_{oc} and FF both fall as temperature rises [3].

For lead halide Perovskite solar cells, the device structure that was been used most frequently is the mesoporous structure, which composed with a hole transporting layer and an electron transporting layer, which often consist with metal oxides, TiO_2. What is in the middle of them, is the light absorbing layer, which is the lead halide perovskite itself. In this kind of solar cell, TiO_2 with different crystal structures were been used in electron transporting layer, for example, anatase and rutile. The difference between rutile and anatase is that rutile has a lower transport efficiency, lower cell voltage, however, longer lifetime.

However, due to the toxicity of lead, the use of lead in electronic devices are restricted, as soon as lead is used in electronic devices and leakage occurs, it will leave serious contaminations to plants and soils. In this case, people are now exploring new lead-free perovskite solar cells, and finally they found that B ion, which is lead ion in the lead halide perovskite can be easily replaced by other ions such as Bi, Ge and Sn, as a result, several kinds of perovskite solar cells has come to people's sights, brought enormous development space and convenience to the research of perovskite solar cells.

2.2. Basic introductions and properties of Tin (II) Perovskite

There are many reasons to choose tin as a replacement of lead acting as a solar cell. Firstly, Sn-based perovskite materials may contain an ABX_3 structure comparable to Pb-based materials since Sn^{2+} and Pb share the same oxidation state. which would have a similar property. Lead and tin both share the same electrical structure since they are members of the same column in the Periodic Table. As a result of their similar electrical and optical characteristics, lead halide and Sn-based perovskites are most likely to behave similarly.

As a substitute for environmental unfriendly Lead Halide Perovskite, Tin Perovskite was one of the strong competitors as it was relatively non-toxic, not so harmful as Lead Halide Perovskite. There were several advantages for Tin Perovskite: Firstly, the crystal structure of Tin Perovskite is similar to the Lead Perovskite, as the ionic radius of Sn and Pb are relatively similar. Secondly, tin perovskites have a really low band gap which were close to the Shockley-Queisser limit, with an outstanding hot carrier lifetime. However, with all of these advantages, the highest power conversion efficiency recorded for tin perovskites was 25.45%, which is a low efficiency compared with lead perovskites. One of the explanations for this low efficiency was tin perovskite's large open-circuit voltage loss [4,5].

This large open-circuit voltage loss could be considered as the poor stability of tin perovskites. In tin perovskite structure, tin (II) can be easily oxidized to tin (IV) under normal air condition, this results in an unacceptable doping concentration, so its efficiency and reproducibility are limited. To increase the power conversion efficiency of tin perovskite, the oxidization of Sn (II) must be stopped to make tin ions more stable. A solvent system could be used to avoid the oxidation by dimethyl sulfoxide. These reducing agents will reduce oxidized Sn (IV) back to Sn (II), such as metal solid Sn or hypophosphorous acid.

$CH_3NH_3SnI_3$ solar cells shows a maximum PCE of 26.92% in a research in 2021. The research measured three different device structures which contains different hole transport material layers. Using the FTO/PCBM/CH3NH3SnI3/CuO device structure, the maximum efficiency results in a value of 25.45%; in the use of TiO_2 in electron transport material layers the best PCE is obtained as 26.92%; and in the case using WO_3 in electron transport material layer, the PCE shows a maximum efficiency of 24.57% under optimum conditions. As Tin ions can be easily oxidized in the working process, the change of temperature can significantly affect the power conversion efficiency of the solar cell: the cell efficiency is reduced when the temperature rises. The effect of temperature was examined in this study from 300 K to 400 K, and the findings indicate that temperature has a significant impact on cell performance. Because photovoltaic properties like bandgap, electron and hole mobility, and carrier concentrations are affected by temperature, cells become less efficient as the temperature rises. This study installed the device in a water-cooling system, which lessens the heating effect and thermal scattering, to ensure that the solar cells functioned well at room temperature. This research proved that $CH_3NH_3SnI_3$ can be used as high efficiency solar cells [6].

For tin perovskite solar cells, using the mesoporous structure has many defects. As the processing of TiO_2 is in a high temperature condition, this will cause tin perovskite to oxidize, result in a low efficiency. To overcome this, tin perovskite has to use a different device structure to allow it working in its maximum power conversion efficiency. A planar structure is now used as the device structure for tin perovskite, with an electron transport layer of fullerenes and hole transport layer of PEDOT: PSS, which can allow the perovskite to work in only low temperature conditions.

2.3. Basic introductions and properties of Germanium Perovskite

Germanium perovskite solar cells were among the perovskites that were one of the most compatible with lead-based solar cells, just like tin perovskite solar cells were. The features of tin, germanium, and lead-based solar cells are comparable since they all fall under the same column of the Periodic Table, as well as having the same electrical configuration and oxidation states. Due to the ease with which Ge^{2+} can be easily converted to Ge^{4+}, Ge-based perovskites share stability difficulties with Sn-based ones.

Several representative examples of germanium perovskite solar cells are $CsGeI_3$, $MAGeI_3$, and $FAGeI_3$, with a band gap of 1.6eV, 1.9eV and 2.2eV. In a research in 2022, $CsGeI_3$ solar cells shows a maximum power conversion efficiency of 10.8%, with a band gap of 1.63eV. In this research, in the highest efficiency dispose, The researchers employed CsGeI3 as an absorb layer with a length of 800 nm and TiO_2 as an electron transport layer, CuI layer as a hole transport layer, and C as the electrode, showing a device structure of FTO/TiO2/CsGeI3/CuI/C. The power conversion efficiency of this model gadget was 10.8%. The research shows that the final PCE can be affected by many factors, for example, temperature, perovskite defect density, interface defect density and perovskite layer thickness.

A homogeneous native oxide surface was produced on $CsSn_{0.5}Ge_{0.5}I_3$, displaying increased stability greater than that of $CH_3NH_3PbI_3$ perovskite, just like tin perovskites due to the highly oxidised properties of Ge (II). According to the study, $CsGeI_3$ has the potential to develop into a useful perovskite solar cell because it can sustain a stable perovskite structure up to 350 °C and yet produce a PCE of 0.11% [7].

2.4. Basic introductions and properties of Double perovskites

A number of fresh halide double perovskites with relatively small bandgaps have been created in recent years as potential Pb-free substitutes for perovskite solar cells [8]. Concluding Double perovskites, usually has a chemical structure of $AA'BB'O_6$, which is based on the structure of single perovskites, ABO_3, where ion A is usually a rare earth element or an alkaline earth element, normally Cs^+, which is similar with that in single perovskite, and differs from single perovskites, ion B' and B'' consist with a cation with an ionic charge of +1 and +3, for example, Ag^+ and Sb^{3+}. Due to the availability of a potentially extremely high number of members and the strong link between magnetic ordering and electronic properties, the mixed-cation double perovskites $AA'BB'O_6$ offer a favorable environment for customizing the needed features.

Double perovskites can be prepared by replacing the Pb cations in Lead Halide Perovskites with a metal cation with an ionic charge of +1 and +3, so its physical structure looks like a arrangement of structures of single perovskites with two different cations. People found that on the basis of the relationship between the two B cations, the chemical structure of double perovskites can have 3 different arrangements: one random arrangement, which also can be written as a formula of $AB'_{0.5}B''_{0.5}O_3$, and two ordered arrangements, Rocksalt Structure and Stratiform Structure.

A long lifespan in carrier recombination, a low effective mass, strong phase stability against humidity, and white-light emission by self-trapped excitons are just a few of the intriguing physical characteristics of double perovskites materials. For example, $Cs2AgBiX_6$ single crystals with improved crystallinity are still in demand for possible applications in a wide range of optoelectronic devices. a comprehensive study was made of the synthesis of highly crystalline $Cs2AgBiX_6$ single crystals in 2020 for these properties [9].

Double perovskites are actually not really suitable in behaving as a solar cell. In research in 2021, a double perovskite solar cell $Cs_2AgBi_{0.75}Sb_{0.25}Br_6$ has made a great progress of a PCE of 18.18%. In this research, spiro-OMeTAD and ZnO are behaving as an HTL and ETL layer between the absorb layer. As a result, the $Cs_2AgBi_{0.75}Sb_{0.25}Br$-based double perovskite solar cell shows an initial power conversion efficiency of 11.35%. After changing the HTL and ETL layer with Cu2O and ZnOS, to get a highest V_{oc} value to maximum the PCE value, the final PCE value is successfully increased to 18.18%. According to the research, the solar cell's device performance is significantly impacted by the perovskite layer's thickness. The photon absorption will rise when the perovskite layer's thickness is increased, that would generate more carriers, so PCE value increases. In this research, the most appropriate thickness for the $Cs_2AgBi_{0.75}Sb_{0.25}Br$ double perovskite is considered as 400 nm [10].

Double perovskites can also be used in the production of solar cells thanks to their phase stability, charge carrier mass, and binding energy. Cs_2SnI_6 is one of the most suitable materials among double perovskites, as it has a band gap of 1.48eV, which is very close to the suitable band gap for the semiconductor in the solar cells, the highest PCE obtained for a double perovskite is 3.11% obtained for $Cs_2AgBiBr_6$ [11,12], which means that double perovskites are not yet suitable in behaving as a solar cell. A farther investigation is needed for double perovskites to make it a more efficient power generation device.

3. Conclusion

This article summarized several kinds of perovskite photovoltaic materials and their performances. It demonstrated that the unique characteristics of perovskite solar cells may truly assist in enhancing the efficiency of power conversion, which is now comparable to that of traditional photovoltaic cells. What's more, perovskite solar cells can be more environmental-friendly and low-cost. In the long run, perovskite solar cells will be a strong competitor to silicon-based solar cells.

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